Sandia National Laboratories

Exceptional service in the national interest

ME469: Numerical Methods and Errors

Stefan P. Domino[1,2]

[1] Computational Thermal and Fluid Mechanics, Sandia National Laboratories

[2] Institute for Computational and Mathematical Engineering, Stanford

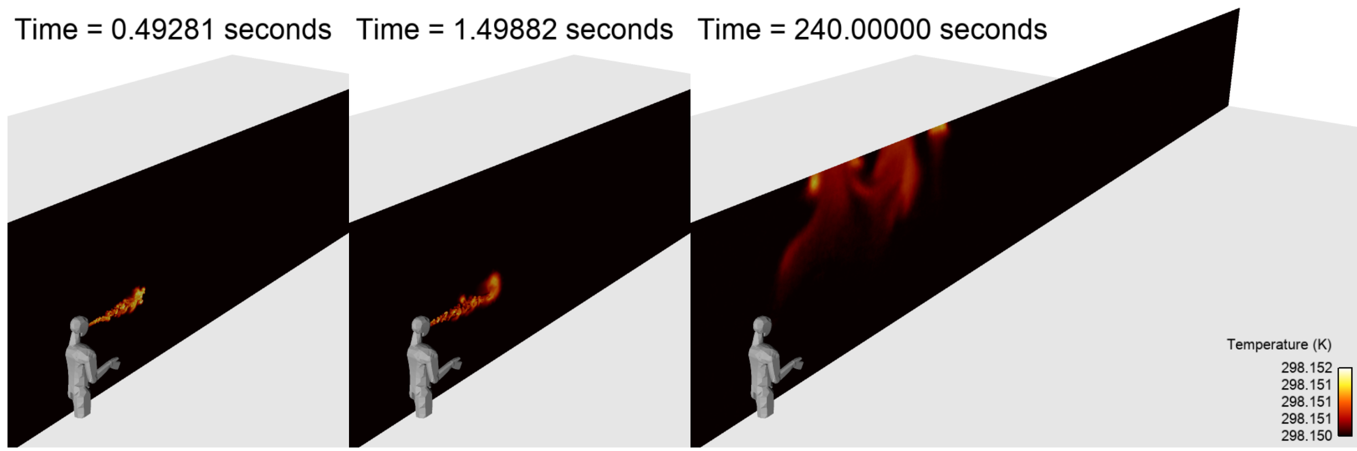
SAND2018-4536 PE

U.S. DEPARTMENT OF ENERGY

NNSA

Simple Passive Scalar Transport

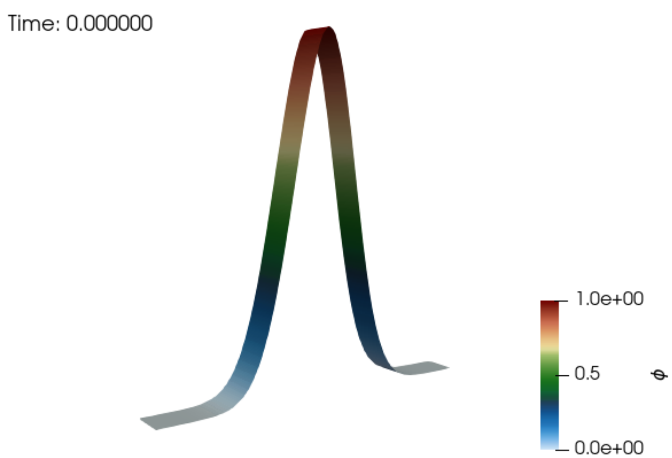
- The study of passive transport of nutrients or pollutants is important in biological and environmental applications (smoke, pathogens, etc.)

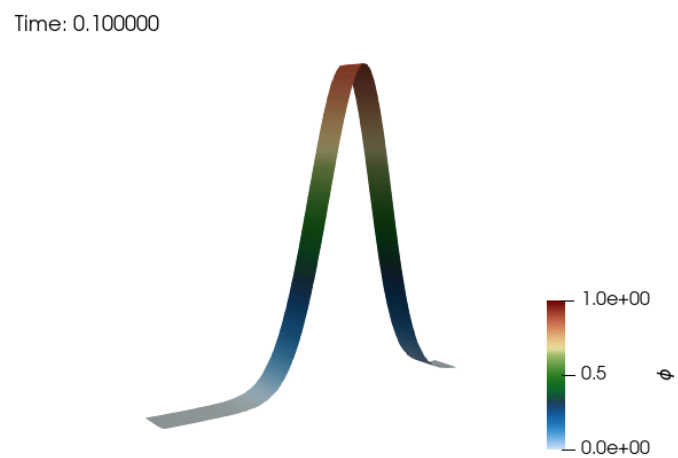


- Left, depicts a passive scalar representing a synthetic cough, Vuorinen et al. "*Modelling aerosol transport and virus exposure with numerical simulations in relation to SARS-CoV-2 transmission by inhalation indoors*", Safety Science (2020)
- Recall that the conceptual model may require buoyancy effects, right, Domino, "*A case study on pathogen transport, deposition, evaporation and transmission: Linking high-fidelity computational fluid dynamics simulations to probability of infection*", Int J. CFD (2021)

One Dimensional Temporal, Advection-Diffusion Equation Passive Scalar Transport

- Let us assume that the problem is defined in a one-dimensional configuration, and that the pollutant concentration is given by, $\phi(x,t)$
- Given an initial distribution of the pollutant $\phi(x,t = T_o)$, we can evaluate the concentration at any later time T_1 through solving a partial differential equation of the form:





$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \nu\frac{\partial^2 \phi}{\partial x^2}$$

Initial Condition:

- Gaussian

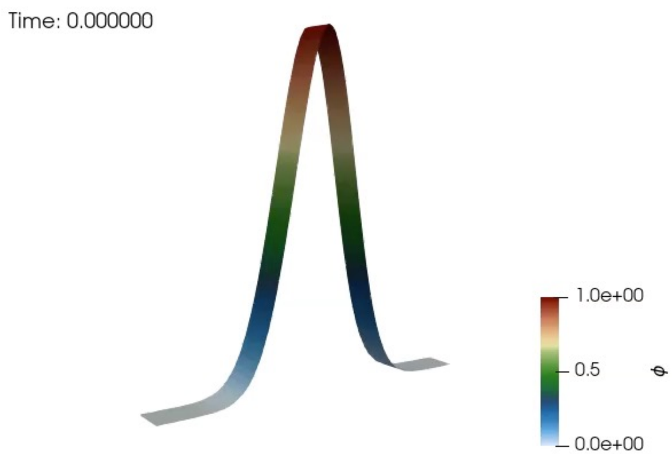
Boundary Condition:

- Domain is periodic

- Above, the air velocity *v* ***is constant***
- Diffusion is characterized by a constant diffusivity ν, ($m^2/2$)

One Dimensional Temporal, Advection-Diffusion Equation
Passive Scalar Transport

- Let us assume that the problem is defined in a one-dimensional configuration, and that the pollutant concentration is given by, $\phi(x,t)$
- Given an initial distribution of the pollutant $\phi(x,t = T_o)$, we can evaluate the concentration at any later time T_1 through solving a partial differential equation of the form:



$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \nu\frac{\partial^2 \phi}{\partial x^2}$$

Initial Condition:

- Gaussian

Boundary Condition:

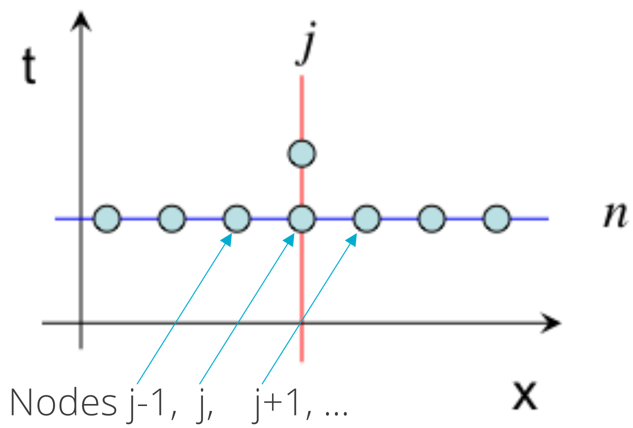
- Domain is periodic

- Above, the air velocity *v* *<u>is constant</u>*
- Diffusion is characterized by a constant diffusivity ν, ($m^2/2$)

The Discretization Step

- The region of interest ($x_L \leq x \leq x_R$) is transformed into a discrete tessellation, i.e. the grid defined by the nodes x_j or the intervals between two nodes (volume) $x_{j+1} - x_j = \Delta x$
- A similar tessellation is also used to represent time discretely in terms of level t_n or intervals $t_{n+1} - t_n = \Delta\tau$
- The solution of the original advection-diffusion equation is only sought at the specific locations (x_j) and time (t_n)

$$\phi(x_j, t^n) = \phi_j^n$$



Approximations to the Continuous Derivative

- The governing equation must also be transformed into an equivalent discrete representation
- The simplest approach involves replacing each (continuous) derivative into a discrete relationship between the function ϕ represented at the grid nodes
- Recall the formal definition of derivative:

$$\frac{\partial \phi(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{\phi(x + \Delta x) - \phi(x)}{\Delta x}$$

- Evaluated for a finite value of Δx

$$\frac{\partial \phi(x)}{\partial x} \approx \frac{\phi(x + \Delta x) - \phi(x)}{\Delta x} \quad (+\epsilon)$$

- Note: The approximate sign represent the effect of the discretization error consequence of a non-zero Δx

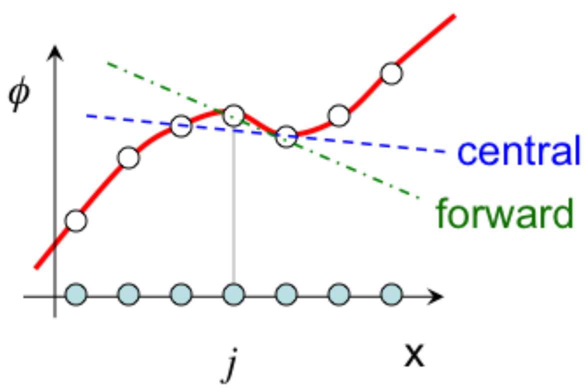
Geometric Interpretation

The formula introduced before,

$$\frac{\partial\phi(x)}{\partial x} \approx \frac{\phi(x+\Delta x)-\phi(x)}{\Delta x}$$

is only one of the possible representations of the derivative

It can be interpreted geometrically as the approximate slope of a smooth interpolant of the discrete values ϕ_j



$$\left(\frac{\partial\phi(x)}{\partial x}\right)_j \approx \frac{\phi_{j+1}-\phi_j}{x_{j+1}-x_j}$$

forward scheme

$$\left(\frac{\partial\phi(x)}{\partial x}\right)_j \approx \frac{\phi_{j+1}-\phi_{j-1}}{x_{j+1}-x_{j-1}}$$

central scheme

Algebraic System of Equations: Explicit

- Starting from the (continuous) mathematical model:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \nu \frac{\partial^2 \phi}{\partial x^2}$$

- The discretization step results in (discrete) computational model, for example using *forward-in-time* and *central-in-space* derivatives:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = \nu \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2}$$

In this case the solution step is straightforward: $\phi_j^{n+1} = F\left(\phi_j^n, \phi_{j+1}^n, \phi_{j-1}^n, v, \nu, \Delta t, \Delta x\right)$

The scheme is **explicit and represents an example of a finite difference technique**

Algebraic System of Equations: Implicit

Different choices of discretization techniques lead to more complex solution steps

- For example, *backward-in-time* and *central-in-space* derivatives: BT-CS

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^{n+1} - \phi_{j-1}^{n+1}}{2\Delta x} = \nu\frac{\phi_{j+1}^{n+1} - 2\phi_j^{n+1} + \phi_{j-1}^{n+1}}{\Delta x^2}$$

- Here, the solution step is formally: $\phi_j^{n+1} = F\left(\phi_j^{n+1}, \phi_{j+1}^{n+1}, \phi_{j-1}^{n+1}, v, \nu, \Delta t, \Delta x\right)$

- Or, better written as a Matrix system: $A\phi^{n+1} = b$

This scheme is **implicit, i.e.,** requires a matrix inversion, **and represents an example of a finite difference technique**

Many Choices on Finite Difference Operators

Central finite difference

Derivative	Accuracy	−5	−4	−3	−2	−1	0	1	2	3	4	5
1	2					−1/2	0	1/2				
	4				1/12	−2/3	0	2/3	−1/12			
	6			−1/60	3/20	−3/4	0	3/4	−3/20	1/60		
	8		1/280	−4/105	1/5	−4/5	0	4/5	−1/5	4/105	−1/280	
2	2					1	−2	1				
	4				−1/12	4/3	−5/2	4/3	−1/12			
	6			1/90	−3/20	3/2	−49/18	3/2	−3/20	1/90		
	8		−1/560	8/315	−1/5	8/5	−205/72	8/5	−1/5	8/315	−1/560	

Forward finite difference

Derivative	Accuracy	0	1	2	3	4	5	6	7	8
1	1	−1	1							
	2	−3/2	2	−1/2						
	3	−11/6	3	−3/2	1/3					
	4	−25/12	4	−3	4/3	−1/4				
	5	−137/60	5	−5	10/3	−5/4	1/5			
	6	−49/20	6	−15/2	20/3	−15/4	6/5	−1/6		

Backward finite difference

Derivative	Accuracy	−8	−7	−6	−5	−4	−3	−2	−1	0
1	1								−1	1
	2							1/2	−2	3/2
	3						−1/3	3/2	−3	11/6

https://en.wikipedia.org/wiki/Finite_difference_coefficient

Properties of Numerical Methods

Outline:

- Consistency
- Stability, Von Neumann Analysis
- Convergence - Lax Equivalence Theorem
- Understanding Errors

High Level Concepts

A discretized mathematical model – a numerical model – is an approximation to the original, postulated, continuous model

- The properties of such numerical model have a strong effect on the computed solution

As a first step we will study three critical properties

- Consistency
- Accuracy
- Stability

Consistency

<u>Definition</u>: A discretization scheme for a mathematical model is <u>consistent</u> if it asymptotes to the original continuous form as the grid and timestep size tend to zero

- *Consistency is a property of the discretization, not of the numerical solution to the given problem*

Q: How to assess if a discretization technique is consistent?

A: Study the truncation error and verify that is vanishes as the grid and timestep size tend to zero.

Stability

Definition: A discretization scheme for a mathematical model is stable if numerical errors (e.g. round-off due to the precision in the computer representation) are not allowed to grow unbounded

- *Stability is a property of the discretization, not of the numerical solution to the given problem*

Q: How to assess if a discretization technique is stable?

A: This is fairly easy for linear PDEs with constant coefficients and no boundary conditions (periodic domains)

Stability Analysis

The simple discretization scheme (FT-CS) for the pure-advection problem is *consistent* but NOT *stable*

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \cancelto{0}{\nu\frac{\partial^2 \phi}{\partial x^2}}$$

Recall it's explicit form:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

Can we understand why and, perhaps, design a different scheme that is stable?

Consistency + Stability Analysis

We can consider the effect of the truncation error as continuous terms in a modified differential equation

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

Applying again a Taylor series expansion and plugging in the expression for the truncation error just found we obtain:

$$\begin{aligned}\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} &= -\frac{\Delta t}{2}v^2\frac{\partial^2 \phi}{\partial x^2} + O\left[(\Delta x)^2, (\Delta t)^2\right] \\ &= -\tilde{\nu}\frac{\partial^2 \phi}{\partial x^2} + O\left[(\Delta x)^2, (\Delta t)^2\right]\end{aligned}$$

- For a given Δx and Δt, note that we are not solving the pure advection equation, although the scheme is consistent (asymptotically)
- Physical viscosity (positive) has the effect of smoothing the solution; but here, the value is negative, and, therefore, **destabilizing**

Convergence

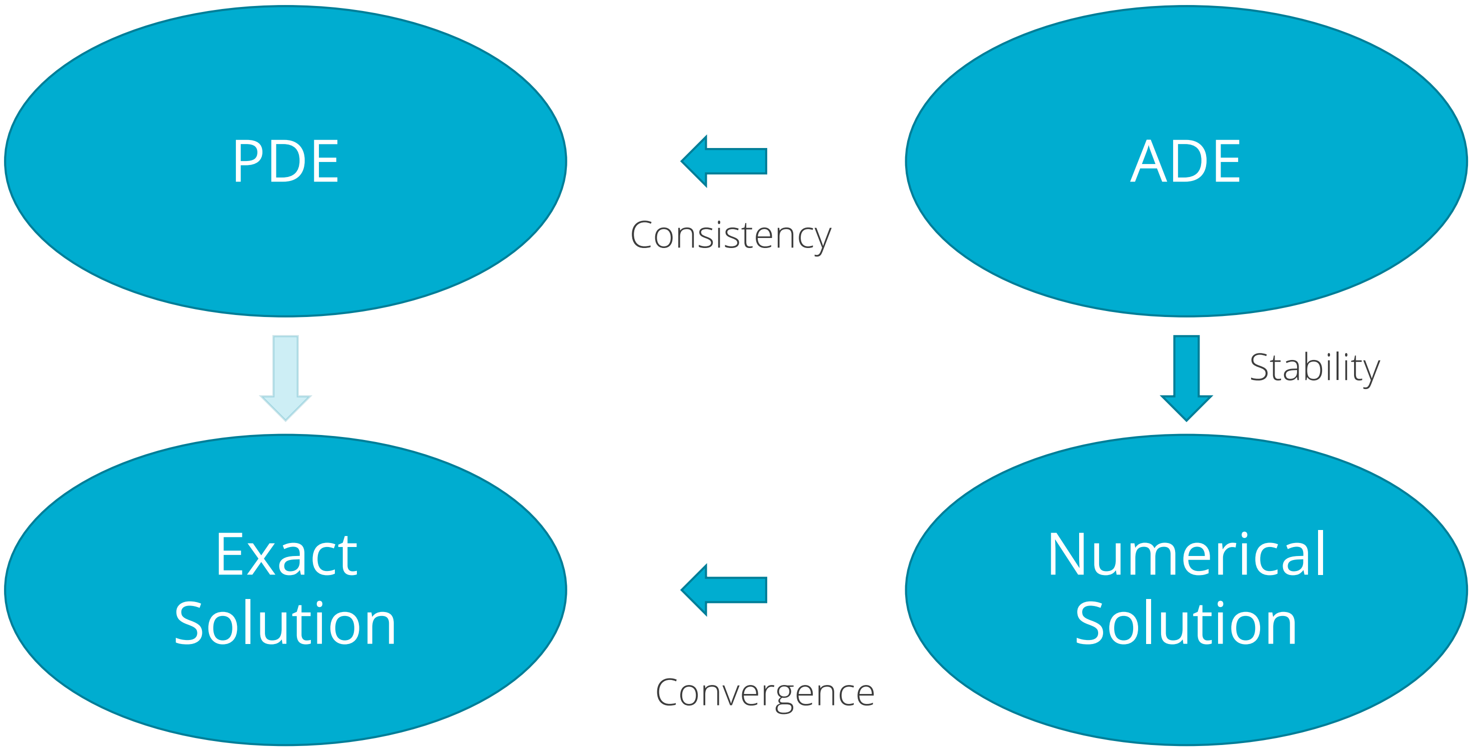
<u>Definition</u>: The numerical solution of a computational model approaches is convergent the exact if it asymptotes to the exact solution of the original continuous problem as the grid and timestep tend to zero

- *Convergence is a property of the solution*

Q: How to assess if the solution is converging?

A: This is formally possible only if the exact solution to the original problem is known!

Numerical Simulation Conundrum



- Convergence is required for a consistent and stable numerical method to recover the exact solution!

Lax Equivalence Theorem

Definition: For a well-posed linear problem discretized using a consistent method, stability is the necessary and sufficient condition for convergence

- In the case of a linear PDE, studying the properties of the computational method is sufficient to know that the exact solution can be computed; even before obtaining any numerical solution!
- For non-linear problems, the analysis is much harder and only weaker statements can be made
- Convergence is studied than directly and in addition to consistency and stability.

Origin of Numerical Errors

Consider again, the pure advection problem:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \nu \underbrace{\cancel{\frac{\partial^2 \phi}{\partial x^2}}}_{0}$$

Recall, the *forward-in-time* and *central-in-space* scheme is consistent but unstable!

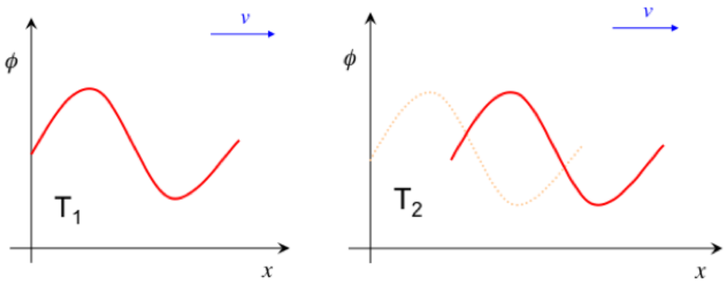
$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

This PDE problem supports an exact solution with a simple physical interpretation

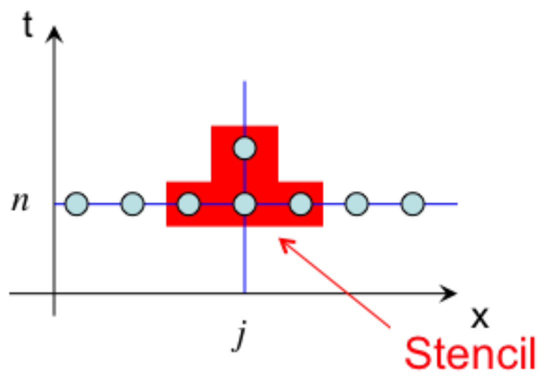
Let's use this finding to gain insight into the behavior of the numerical scheme

Evaluating the Exact Advection Equation Solution

Physical Interpretation: Information travels in the v-direction (positive)



Numerical Method: However, information is gathered from both j-1 and j+1 states



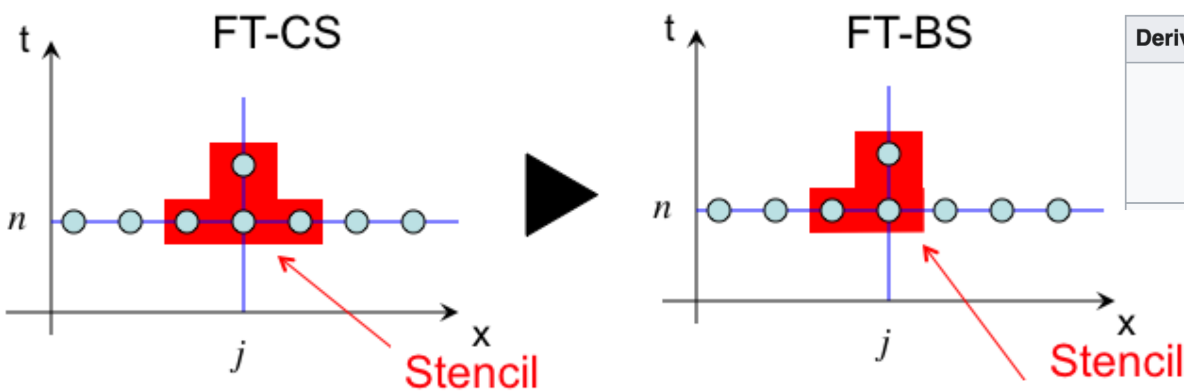
$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

Exploiting the Directionality of the Flow

An alternative choice of spatial discretization provides a more physically-consistent discrete model: for example, if flow is moving from left to right, let's remove the j+1 contribution

- Consider a *forward-in-time* and *backward-in-space* differentiation (FT-BS)

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} = 0$$



Recall backward finite difference stencil

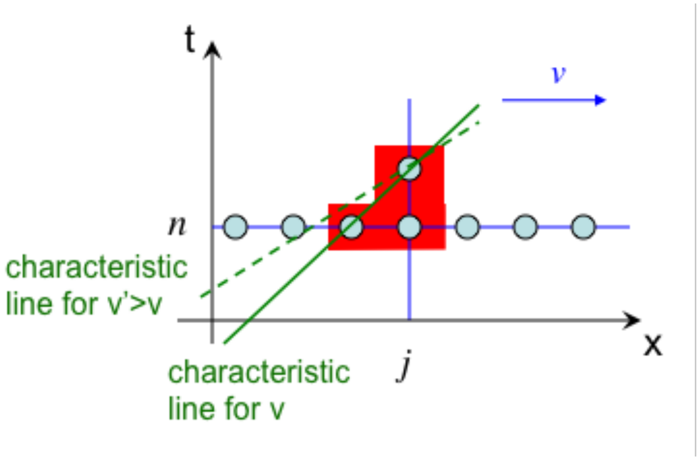
Derivative	Accuracy	−8	−7	−6	−5	−4	−3	−2	−1	0
1	1								−1	1
	2							1/2	−2	3/2
	3						−1/3	3/2	−3	11/6

- This scheme is consistent and conditionally stable (see course reader) using Von Neumann stability analysis that shows |amplification factor| is less than unity when $\dfrac{v\Delta t}{\Delta x} \leq 1$

Properties of the FT-BS

The scheme is consistent and conditionally stable. Why?

The characteristics lines (for fixed Δx and Δt provide the physical picture:



Deriving the modified equation leads to a clear understanding of an underlying stabilization mechanism….

Modified Equation for the Forward-in-time, Backward-in-space

The FT-BS scheme is equivalent to:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \frac{v}{2\Delta x}\left(\phi_{j+1}^n - \phi_{j-1}^n\right) = \frac{v\Delta x}{2}\left(\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2}\right)$$

and results in the modified equation:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \frac{v\Delta x}{2}\frac{\partial^2 \phi}{\partial x^2}$$

- The backward-in-space discretization leads to a positive dissipation, e.g. a stabilization of the scheme
- However, what happens if *velocity* < 0?

Introducing: An Upwind-based Scheme

Is it possible to simply switch between FT-BS (v > 0) and FT-FS (v < 0), while ensuring that the scheme is *consistent* and *conditionally* stable?

First, let's define an upwind and downwind operators:

$$v^{+} = \frac{v + |v|}{2} \qquad v^{-} = \frac{v - |v|}{2}$$

Furthermore, let's provide a general upwind scheme system as:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v^{+} \frac{\phi_j^n - \phi_{j-1}^n}{\Delta x} + v^{-} \frac{\phi_{j+1}^n - \phi_j^n}{\Delta x} = 0$$

That can be reorganized as:

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \frac{v}{2\Delta x} \left(\phi_{j+1}^n - \phi_{j-1}^n\right) = \frac{|v|\Delta x}{2} \left(\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2}\right)$$

Modified Equation for the Upwind-based Scheme

Recall,

$$\frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + \frac{v}{2\Delta x}\left(\phi_{j+1}^n - \phi_{j-1}^n\right) = \frac{|v|\Delta x}{2}\left(\frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{\Delta x^2}\right)$$

and results in the modified equation:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \frac{|v|\Delta x}{2}\frac{\partial^2 \phi}{\partial x^2}$$

The above form provides stabilization that is positive for all real values of velocity

Stability can also be studied using Von Nuemann analysis and results in the constraint that:

$$\frac{|v|\Delta t}{\Delta x} \leq 1$$

General Notes

- The consistency analysis and the derivation of the modified equation clearly illustrate the impact of numerical errors on the problem being solved
- The derivation of the upwind scheme shows that dissipation-like errors lead to stabilization
- What other errors can we expect to see using different discretization schemes?
- Let's re-visit the FT-CS advection system:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} = \nu \cancelto{0}{\frac{\partial^2 \phi}{\partial x^2}} \longrightarrow \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + v\frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta x} = 0$$

- The truncation error for the FT-CS scheme is:

$$\epsilon = -\frac{\Delta t}{2} v^2 \left(\frac{\partial^2 \phi}{\partial x^2}\right)_j^n - v\frac{\Delta x^2}{6}\left(\frac{\partial^3 \phi}{\partial x^3}\right)_j^n + O\left[(\Delta x)^2, (\Delta t)^2\right]$$

- Let's examine each separately

Model 1 and Model 2 Modified Equations

Model 1:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} - \alpha\frac{\partial^2 \phi}{\partial x^2} = 0$$

Model 2:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} + \beta\frac{\partial^3 \phi}{\partial x^3} = 0$$

Objective: Find the exact solution to these model equations in a simple periodic domain

Model 1

Postulate an expression for the solution: $\phi(x,t) = e^{pt}e^{ikx}$

Plug in the PDE: $\dfrac{\partial \phi}{\partial t} + v\dfrac{\partial \phi}{\partial x} - \alpha\dfrac{\partial^2 \phi}{\partial x^2} = 0$

to obtain $pe^{pt}e^{ikx} + ivke^{pt}e^{ikx} + \alpha k^2 e^{pt}e^{ikx} = 0$

This is satisfied if $p = -ivk - \alpha k^2$, leading to the solution:

$$\phi(x,t) = e^{(-ivk-\alpha k^2)t}e^{ikx} = e^{ik(x-vt)}e^{-\alpha k^2 t}$$

Model 1

Postulate an expression for the solution: $\phi(x,t) = e^{pt}e^{ikx}$

Plug in the PDE: $\dfrac{\partial \phi}{\partial t} + v\dfrac{\partial \phi}{\partial x} - \alpha \dfrac{\partial^2 \phi}{\partial x^2} = 0$

to obtain $pe^{pt}e^{ikx} + ivke^{pt}e^{ikx} + \alpha k^2 e^{pt}e^{ikx} = 0$

This is satisfied if $p = -ivk - \alpha k^2$, leading to the solution:

$$\phi(x,t) = e^{(-ivk-\alpha k^2)t}e^{ikx} = e^{ik(x-vt)}e^{-\alpha k^2 t}$$

Model 2

Postulate an expression for the solution: $\phi(x,t) = e^{pt}e^{ikx}$

Plug in the PDE: $\dfrac{\partial \phi}{\partial t} + v\dfrac{\partial \phi}{\partial x} + \beta\dfrac{\partial^3 \phi}{\partial x^3} = 0$

to obtain $pe^{pt}e^{ikx} + ivke^{pt}e^{ikx} - \beta ik^3 e^{pt}e^{ikx} = 0$

This is satisfied if $p = -ivk + \beta ik^3$, leading to the solution:

$$\phi(x,t) = e^{(-ivk+\beta ik^3)t}e^{ikx} = e^{ik[x-(v-\beta k^2)t]} = e^{ik(x-wt)}$$

Model 2

Postulate an expression for the solution: $\phi(x,t) = e^{pt}e^{ikx}$

Plug in the PDE: $\dfrac{\partial \phi}{\partial t} + v\dfrac{\partial \phi}{\partial x} + \beta\dfrac{\partial^3 \phi}{\partial x^3} = 0$

to obtain $pe^{pt}e^{ikx} + ivke^{pt}e^{ikx} - \beta ik^3 e^{pt}e^{ikx} = 0$

This is satisfied if $p = -ivk + \beta ik^3$, leading to the solution:

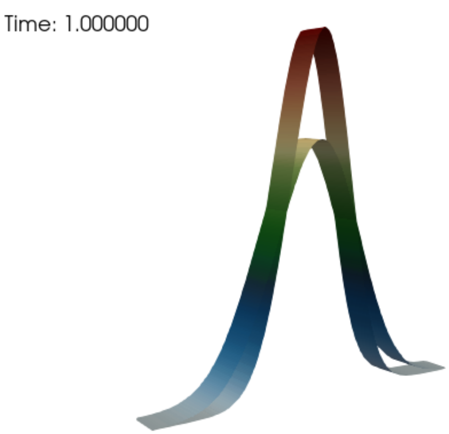
$$\phi(x,t) = e^{(-ivk+\beta ik^3)t}e^{ikx} = e^{ik[x-(v-\beta k^2)t]} = e^{ik(x-wt)}$$

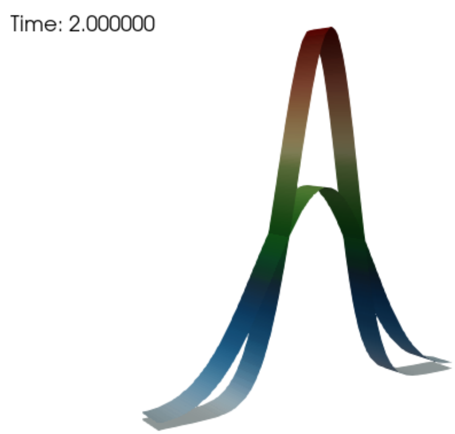
Model 1: Dissipative-like Error

Review:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} - \alpha\frac{\partial^2 \phi}{\partial x^2} = 0$$

$$\phi(x,t) = e^{(-ivk-\alpha k^2)t}e^{ikx} = e^{ik(x-vt)}e^{-\alpha k^2 t}$$



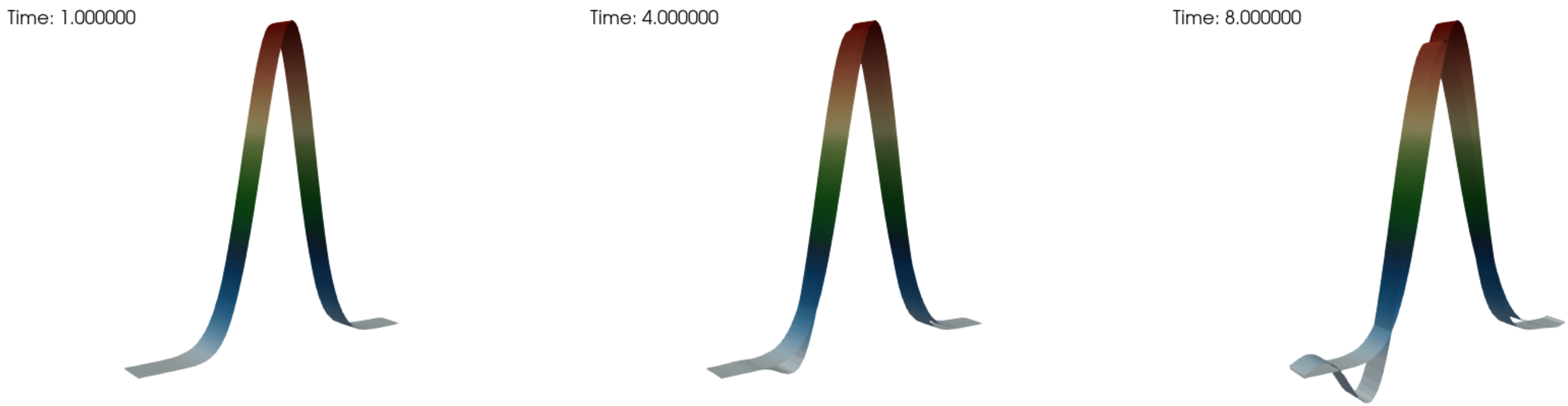


Model 2: Dispersion-like Error

Review:

$$\frac{\partial \phi}{\partial t} + v\frac{\partial \phi}{\partial x} + \beta\frac{\partial^3 \phi}{\partial x^3} = 0$$

$$\phi(x,t) = e^{(-ivk+\beta ik^3)t}e^{ikx} = e^{ik[x-(v-\beta k^2)t]} = e^{ik(x-wt)}$$

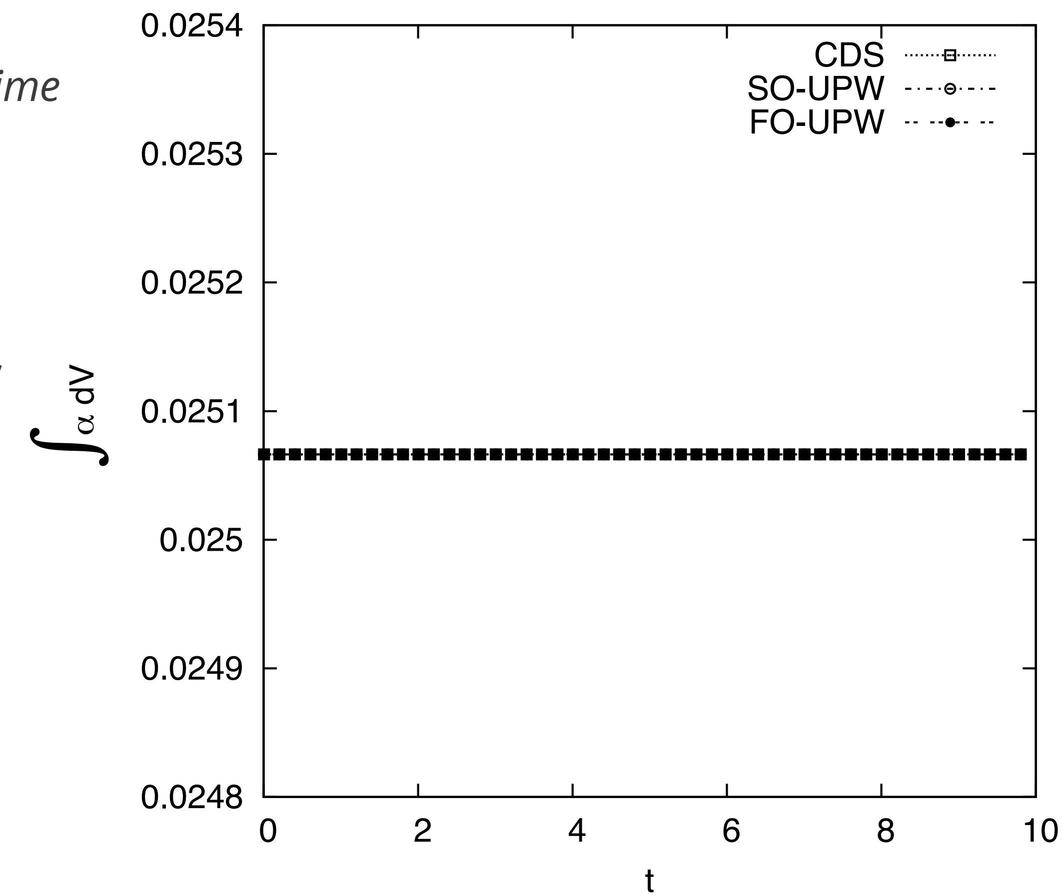


A Note on Conservation: ϕ

For our fully implicit *backward-in-time* and *central-in-space* Nalu finite volume approach:

Integration ϕ over the full domain, for any advection operator choice, results in:

- Perfect conservation

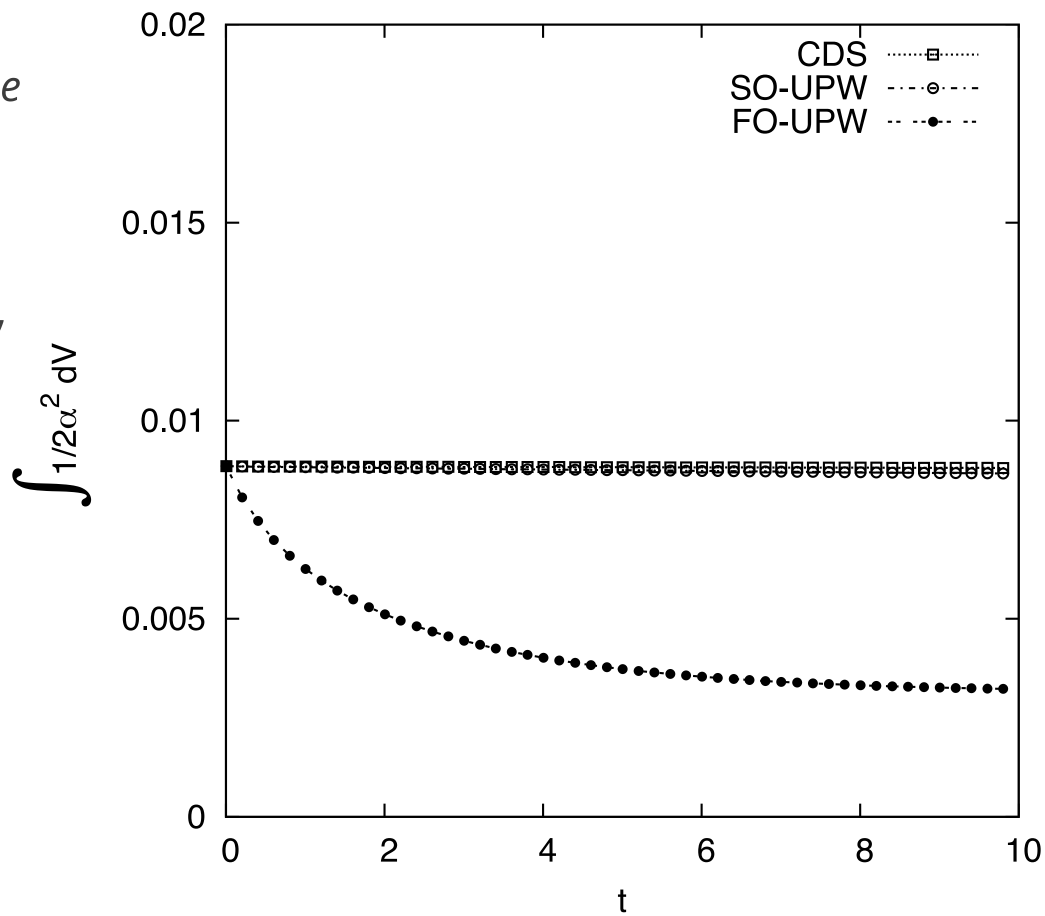


A Note on Conservation: $\phi^2/2$

For our fully implicit *backward-in-time* and *central-in-space* Nalu finite volume approach:

Integration $\phi^2/2$ over the full domain, for any advection operator choice, results in:

- Lack of conservation for the upwinded approaches
- Ideal conservation for the central operator
- Energy-method where the PDE is derived for the energy-variable, see course reader



Final Notes

- Studying the numerical properties of the discretization technique is critical to set the proper expectations on the solutions
- Classical tools such as Von Neumann stability analysis are easy to use but not generalizable
- Other properties (beyond consistency, stability, etc.) can be critical.
  - We will introduce *conservation*, *boundedness* and *symmetry*.
- Good understanding of the physics of the problem leads to better choices for the numerical schemes